Optimal mechanical performance prediction of a sediment-based geopolymer road sub-layer

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ABSTRACT: In a world where concrete is king and because of the environmental challenges, it is urgent to find sustainable alternatives to the latter. From this perspective, this study considers the replacement of concrete with raw materials, namely sediments. Precisely, this work aims to predict the compressive strength of geopolymer mortars made from sediments. The approach combines principal component analysis (PCA) and ordinary least squares (OLS) multivariate regression models. The predictive model highlights several indicators, such as clay, specific surface, and sediment density. Other indicators, such as organic matter and geopolymerization activators, should be considered, although not statistically significant.

Driven by the evolution of the global environmental context, public works must rethink their sector towards more sustainable applications. Numerous research in France focuses on the development of alternative materials in construction. Dredged sediments are a significant source of interest among these materials due to their large volume. Therefore many emerging projects in France demonstrate the ability to use dredged sediments in several civil engineering applications: bricks (Serbarh et al., 2018), concrete pavements (Limeira et al., 2010) and lightweight concrete (Abdallah et al., 2019). Reusing sediments as a component in concrete offers both environmental and economic benefits. However, one of the challenges in using dredged sediments is their variable mineralogical properties. Nevertheless, its use in the manufacture of geopolymer binders proves to be an innovative solution for their recovery and could allow the emergence of a new ecological binder to replace Portland cement.

Models for predicting the 28-day compressive strength of concrete containing dredged sediments have been assessed in the literature. Among them, Chu and al. (2020) developed a strength model with a multi-variable methodology to correlate mechanical strength to design parameters such as the volumetric ratio of dredged sediments and cement paste volume. A predictive equation was developed, which allowed a better comprehension of the direct use of sediments; yet, the model was simplified by assuming similar physical and chemical properties for the sediment used. Other approaches, such as the one developed by Tran and al. (2021), show artificial intelligence's ability to predict the mechanical strength of stabilized dredged sediments by only considering design parameters. One of the few studies that linked raw sediment's design parameters and properties was the one developed by Moghrabi et al. (2018). Based on a statistical study, an estimation of the comprehensive strength at 28 days was established and showed the detrimental influence of the organic matter content and plasticity index of sediment on mechanical strength.

To date, few studies are predicting the influence of sediment, taking into account their physicochemical variability, on the properties of concrete and, to the author's knowledge, none of them were dealing with geopolymer matrix. Thus, the objective of the present paper is to predict the mechanical performance of a sediment-based geopolymer road sub-layer by taking into account the variability of the raw sediments used. The developed model will highlight the effects of various parameters on the mechanical strength and obtain a better comprehension of the geopolymer matrix with untreated dredged sediment. Furthermore, results will be transposed to an existing road sub-layer model to develop a probabilistic model for predicting mechanical performance. On a larger scale, this paper aims to facilitate the valorization of dredged sediment, which is currently hindered due to the difficulty of developing a robust predictive model for sediment-based concrete performance.

1. METHODOLOGY

1.1. Materials and mixed design

1.1.1. Sampling campaign

Eight sediment samples were chosen from four different Harbors in the Gironde region from the South West of France. Pauillac (PAU) refers to the sediment obtained from a dredging campaign by The Bordeaux Harbor in the Gironde estuary. Four sediments were collected from different landfill deposits owned by Arcachon Bay. Arcachon's sediments are referred to as Audenge (AUD), Quiconce (QUIN), Titoune (TIT) and LeTeich (LETEI). BY1 and BY2 were dredged in Bayonne Harbor and LR in La Rochelle Harbor.

1.1.2. Characterization

In this study, muddy sediments were chosen, given their limited valorization in actual research. The physical properties of sediment samples have been compared and are presented in Table 1. Particle size distribution, density, Atterberg limits, clayey and organic content were evaluated according to the French Standards. Characterization results show that the sampled sediments present similar physical properties, even if distinctions can be observed. Concerning the granular distribution, clay percentage can range from 0.72% for AUD to 5.35% for TIT, with a total medium value of 2.6%. Silty content is the highest for QUIN (56.53%) and lowest for LR (35.21%), whereas sand content varies from 5.69% for TIT and 26.74% for LR. Particle size distributions of the sediments are presented in Figure 1. High plasticity indexes are observed for BY1 and low for QUIN. As well as for the organic content, sediments sampled in the same Harbor do not present the same value, especially when observing the sediments from Arcachon Harbors.

Table 1: Physical properties of the sediments.

	PAU	**AUD**	**QUIN**	**TIT**
Clay [%]	2.93	0.72	1.44	5.35
Fine silts [%]	23.15	22.89	36.09	41.08
Coarse silts [%]	23.15	18.26	20.44	13.09
Fine sand [%]	10.76	10.07	5.87	4.06
Coarse sand[%]	0.43	13.32	1.37	1.63
Blaine [m^2/g]	0.65	0.16	0.43	00.48
Density [$g.cm^{-3}$]	1.45	1.57	1.24	1.35
Ip [%]	25.75	19.00	16.00	42.24
VBS [$g.100g^{-1}$]	2.80	1.55	1.7	1.13
OM [$mg.kg^{-1}$]	10500	2466	34300	41000
	LETEI	**BY1**	**BY2**	**LR**
Clay [%]	0.94	2.88	3.14	3.26
Fine silts [%]	25.77	21.78	24.26	22.17
Coarse silts [%]	16.21	18.72	21.00	13.04
Fine sand [%]	9.84	12.21	10.61	18.91
Coarse sand[%]	12.45	9.61	6.19	7.83
Blaine [m^2/g]	0.38	0.49	0.48	0.37

ρ [$g.cm^{-3}$]	1.70	1.30	1.34	1.72
Ip [%]	41.00	61.00	49.50	48.00
VBS [$g.100g^{-1}$]	3.00	1.67	1.00	4.67
OM [$mg.kg^{-1}$]	41000	37100	39600	3790

Regarding chemical properties, the elemental composition obtained by Scanning Electron Microscopy was investigated in this study in addition to the associated minerals obtained with X-Ray Diffraction. The studied sediments are mainly aluminosilicate materials which justify their use in geopolymer matrix as a precursor. The chemical properties of sediments are presented in Table 2.

Table 2: Chemical properties of the sediments.

	PAU	AUD	QUIN	TIT
Al_2O_3 [%]	14.19	15.91	21.27	16.81
SiO_2 [%]	41.38	54.25	58.76	51.91
SiO_2/ Al_2O_3	2.92	3.41	2.76	3.09
	LETEI	**BY1**	**BY2**	**LR**
Al_2O_3 [%]	15.34	15.94	12.97	11.06
SiO_2 [%]	44.75	49.93	46.63	25.44
SiO_2/ Al_2O_3	2.92	3.13	3.59	2.30

1.1.3. Mix design

Previous studies conducted by the authors have sought to use sediments as a precursor in the geopolymerization process regarding their aluminosilicate nature. Following the work made by Monteiro and al. (2022) and in order to observe the influence of the sediment properties on the final mechanical strength of a sediment-based geopolymer sub-layer, a unique optimal formulation was fixed.

The production of geopolymerized mortar from dredged sediments is based on the reaction between 70% of untreated sediment at a water content of 30% with 30% alkali reagent by mass. The alkali reagent mixture is a combination of a 4 $mol.L^{-1}$ solution of NaOH and Na_2SiO_3 with an optimum weight ratio of SiO_2/Na_2O solution of 1.2. Sodium hydroxide (NaOH) was used in the form of pellets (99% purity) which were dissolved in a ready-to-use silicate solution (Na_2SiO_3). The volume and the water/solid ratio are kept constant at 1 m^3 and 0.40, respectively. The specimens, 4x4x16 cm^3 in size, were vibrated with a vibrating table, removed from the mold after 24 hours and then stored in a room maintained at relative humidity and a respective temperature of RH=60% and T=20°C for 28 days. Compressive strength measurements were carried out according to French standard NF EN 1015-11 with an electromechanical press capacity of 100 kN at a constant loading speed of 0.6 mm/min at 28 days.

1.2. Statiscal approach

This section defines the statistical approach to link the sediments' physicochemical parameters with the experimentally obtained compressive strength. Two methods were used: Principal Component Analysis (PCA) and Ordinary Least Square (OLS) regressions. Methods are developed below.

1.2.1. Principal Component Analysis (PCA)

PCA is a quantitative data analysis method based on multidimensional exploratory statistics. The "exploratory" term refers to the descriptive side of the method, as opposed to inferential statistics, which consists of generalizing results to an entire population by formalizing statistics risk thresholds. The "multidimensional" term refers to the simultaneous study of a complex data table, where *I* individuals are represented in lines, and *K* variables are represented in columns.

PCA is used here to represent both Table 1 and Table 2 in the simplest way possible. The idea is to have an appropriate and simplified image of all the points given by the cloud of points or *I-K* matrix. Methodologically, from a large dataset of *K*-correlated variables, PCA creates uncorrelated components "where each component is a linear weighted combination of initial variables" (Vyas & al., 2006). Euclidean geometry calculates the distance between individuals to know their multidimensional resemblance. In practice, data must first be centered and reduced to implement this method.

Thus, the cloud of points is projected on a minimum of axes called "components" (deforming it as little as possible), spreading it as much as possible on the projection planes. The idea is to search for a series of orthogonal axes of maximum inertia (defined as the squares' sum of the distances of the points from the center of gravity). Ultimately, it is known that the correlation matrix admits eigenvalues and eigenvectors. The solution is to diagonalize this correlation matrix where eigenvectors give the weight of each principal component and eigenvalues represent the variance of each principal component (the maximum of projected inertia). Finally, each component will explain one part of the initial database variance, but explanations will be progressively less efficient as the components are retained.

The "images" of statistical reality, obtained according to the principles set out above, are only images reflecting this reality "at best". Therefore, it is necessary to establish figures allowing the results to be interpreted rigorously and appropriately. According to the previous remark, three main tools help with the interpretation. First, the quality of the cloud's representation by an axis helps measure the percentage of the total statistical information captured by a projection axis. Second, the quality of an element's representation by an axis helps measure the percentage of the statistical information carried by the element considered, which is captured by the axis considered. Third, the contribution of an element to the inertia of an axis helps measure the percentage of the statistical information carried by the axis considered, which is attributable to the element considered.

1.2.2. Ordinary Least Square (OLS)

In the second part, a linear regression model is used to explain the dependent variable, which is the compressive strength (R_C) as a function of a set of other variables (called explanatory variables) by quantifying a single equation:

$$R\_Ci = \sum_{i=0}^{N} \beta_0 \pm \beta_1 X_1 \pm \beta_n X_n \pm \varepsilon_i \qquad (1)$$

where R_Ci, X_i and ε_i are the *ith* observation of the dependent variable, the independent variable, and the error term, respectively; the estimators β are the regression coefficients; and N is the number of observations.

Three main reasons drive the choice to use an OLS estimation technique. First, this estimator is relatively easy to use. Second, as the studied relationship is supposed to be linear, the goal of minimizing the summed squared residuals is entirely appropriate from a theoretical point of view. Finally, this estimator has several valuable properties as the sum of the residuals is precisely zero, and it is the "best" estimator possible under a set of specific assumptions that should be checked here. The OLS method is BLUE (best linear unbiased estimate) if five assumptions are verified:

1. Linearity of the relationship between the parameters studied.
2. $E(\varepsilon_i|X_n) = 0$: Exogeneity between regressors and the error term.
3. Absence of colinearity between regressors (not perfectly correlated with each other).
4. $\mathrm{Var}(\varepsilon_i|X_n) = \sigma^2$: Homoscedasticity of the variance (that means the error of the variance is constant).
5. Use of data that are randomly sampled from the population.

2. RESULTS

2.1. Compressive Strength

As illustrated in Figure 4 further in the text, the compressive strength results of the eight tested individuals range from 3.64 MPa for TIT to 0.31 MPa for AUD. Therefore, sediments from different places with different parameters and explanatory variables can lead to different results when using a similar formulation. A statistical approach will be used in the following parts to observe the main determinants of compressive strength variation between individuals. In other words, the objective is to determine the influence of sediments, more precisely their properties, on mechanical resistance.

2.2. PCA results

The PCA analyzes the eight individuals through 14 parameters referring to their physical and chemical properties (Table 1 and Table 2). PCA's first approach involves studying individual variability, as illustrated in Figure 1.

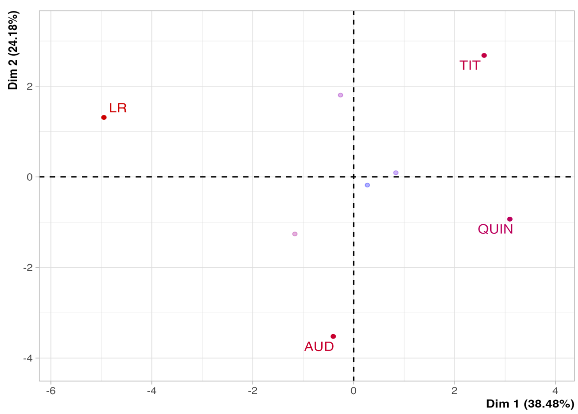

Figure 1: PCA graph of individuals.

The first two components of PCA are retained in this figure to have a simple two-dimensional picture of individuals, accounting for 62.66% of the total dataset inertia and their representation quality (see the color's intensity for cos2 graphically). The first axis demonstrates an opposition between TIT and QUIN (to the right of the graph, characterized by a strongly positive coordinate on the axis) to LR (to the left of the graph, characterized by a strongly negative coordinate on the axis). Precisely, TIT and QUIN are similar by sharing a high value for Blaine and low values for Density and Coarse sand. In opposition, LR is characterized by high values for VBS and Fines sand and low values for Density and Coarse sand. As part of the second axis, it distinguishes individuals such as AUD (to the bottom of the graph, characterized by a strongly negative coordinate on the axis) sharing high values for the Coarse sand variable.

Besides, Figure 2 and Figure 3 describe the second approach of PCA that establishes links between the 14 parameters studied to synthesize them. As previously seen (in section 1.2.1), the results presented are selected according to the respective contribution of parameters to the inertia of axes and their representation quality. Components retained should represent a high variability in initial multidimensional data. The criterion is generally to retain components with eigenvalues greater than 1. Here, the first three acomponents are retained, which is already satisfying, accounting for 76.43% of the total dtaset inertia.

In Figure 2, the first component opposes Fine silts, Al_2O_3, and SiO_2 (positive coordinates on the axis) to Fine sand, Density, and VBS (negative coordinates on the axis). The second component traduces the opposition between R_C, Clay, and Blaine (positive coordinates on the axis) to Coarse sand (negative coordinates on the axis). Finally, in Figure 3, the third component illustrates the opposition between Ip, SiO_2/Al_2O_3, and OM (positive coordinates on the axis) with Fine silts, Al_2O_3, and VBS (negative coordinates on the axis).

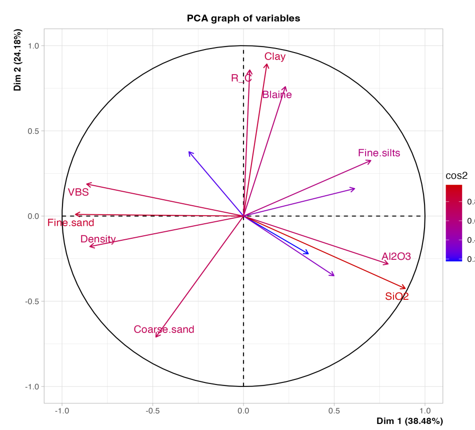

Figure 2: PCA graph of Figure variables representing the first two components.

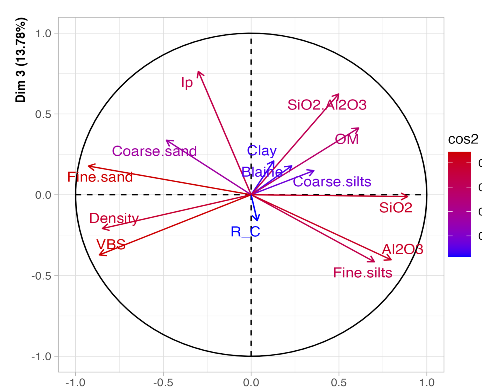

Figure 3: PCA graph of Figure variables representing the first and third components.

2.3. OLS results

In this section, the objective is to predict the mechanical performance (R_C) of the different raw sediments collected. The results in Table 3 show p-values of statistically significant causal relationships between the independent parameters tested and the explained variable (R_C). Different potential determinants of R_C are tested. First, Clay and Blaine are strongly correlated to R_C according to the second component of the PCA analysis. Knowing that correlation is not a synonym for causality but can highly indicate its potential presence, Model 1 of Table 3 tests these parameters.

Following Chu and al. (2020) highlighting the importance of the volumetric ratio of dredged sediments for mechanical strength, the Density parameter is added in Model 2. Models 3 and 4 test the causal impact of Ip and OM parameters on R_C. Indeed, these parameters are presented as determinants by Moghrabi et al. (2018) and appear essential in the third component of the PCA analysis. Finally, Models 5 and 6 investigate the impact of sediments' chemical properties which are Al_2O_3 and SiO_2. The best predictions for R_C are obtained in Models 3 and 6, which have a very satisfying adjusted R-squared of 87.1% and 98.8%, respectively.

These coefficients of determination tell how much variation in the dependent variable can be explained by the independent variables tested and are very satisfying. Moreover, the F-statistic tells the regression's goodness of fit, indicating the pertinence of selected parameters. According to these best models, three main significant parameters influence R_C, which are Blaine (at a 5% level of confidence), Density (at 10%), and Clay (at 5%). More precisely, in Model 6, which is the best, a unit change in Blaine rises R_C by 7.184, 7.112 for Density, and 0.903 for Clay. We also partially validate the results of Moghrabi et al. (2018) by showing that Ip and OM negatively impact mechanical strength, although these parameters are statistically non-significant here. Concerning SiO_2, it also seems positively impact R_C but is non-significant too. Although non-significant, Ip, OM, and SiO_2 appear as important variables to control for, expected to play a role in R_C prediction and increase the model's power. Thanks to the Model 6 retained, R_C can be predicted with confidence, as seen in Figure 4.

Table 3: OLS results with regression coefficients (8 individuals).

VARIABLES	Model1 R_C	Model2 R_C	Model3 R_C	Model4 R_C	Model5 R_C	Model6 R_C
Clay	0.550**	0.580*	0.819**	0.832**	0.832	0.903**
	(0.209)	(0.242)	(0.151)	(0.147)	(0.208)	(0.0308)
Blaine	2.597	4.027	4.425**	4.388	4.397	7.184**
	(3.587)	(3.708)	(1.290)	(1.791)	(2.676)	(0.558)
Density		2.686	3.527*	3.793*	3.806	7.112*
		(1.656)	(1.359)	(1.279)	(1.979)	(0.744)
Ip			-0.0440**	-0.0467	-0.0465	-0.0243
			(0.00975)	(0.0164)	(0.0284)	(0.00605)
OM				4.91e-06	4.76e-06	-1.74e-05
				(1.42e-05)	(2.43e-05)	(5.24e-06)
Al_2O_3					0.00180	
					(0.163)	
SiO_2						0.0902
						(0.0163)
Constant	-1.029	-5.640	-5.993*	-6.425	-6.481	-17.12*
	(1.094)	(3.257)	(2.377)	(2.540)	(5.622)	(2.108)
Observations	8	8	8	8	8	8
Adjusted R-squared	0.495	0.558	0.871	0.814	0.628	0.988
F-Stat	822.2	822.2	822.2	822.2	822.2	822.2
Prob > F	0.0267	0.0267	0.0267	0.0267	0.0267	0.0267

Robust standard errors in parentheses: *** p<0.01, ** p<0.05, * p<0.
Source: author's calculations.

These results satisfy previously announced OLS assumptions in section 1.2.2 to have an unbiased estimator. First, R_C can be estimated through a linear relationship. Second, essential regressors are included in regression analysis to avoid approaching a zero error term. Third, colinearity between regressors is studied through VIF analysis (Variance Inflation Factor) in Table 3. In parallel, the OLS method must satisfy two conditions to be the most optimal and precise estimator. Concerning that fact, robust variance estimates are proposed in the results to control for potential homoscedasticity issues. Finally, data should be randomly sampled from the population, and the sample size should be sufficient (N>30) to guarantee a normal data distribution and use the Central Limit Theorem (CLT). The sample is very limited to satisfy this condition, and the data are not entirely normally distributed.

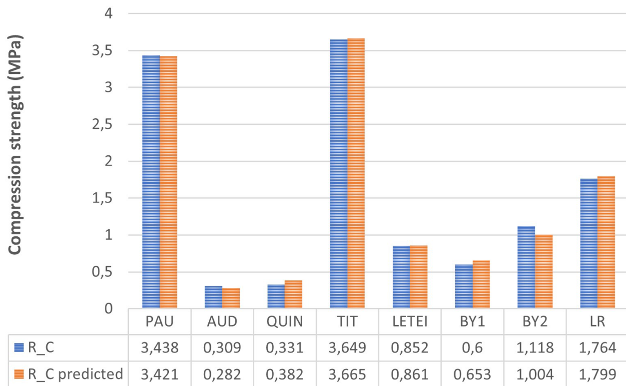

Figure 4: Comparison between actual measurements of R_C and predictions.

2.4. Extension to OLS results

One noting fact with these results is the absence of water, sediment, and alkali reagents as significant determinants of R_C. These results are not surprising given the construction of these eight sediment samples, all coming from Pauillac as explained in part 1.1.1 and based on the better mixture obtained from 27 individuals (see section 1.1.3). Hence, for the eight individuals previously studied, parameters such as H_2O, NaOH, and Na_2SiO_3 are considered constant (fixed for a mixture volume equal to 1). An extension to the research question of this article could be the study of parameters that more broadly influence R_C, using these 35 individuals in total. These results are presented in Table 4. The best predictions are obtained in Models 3 and 4, which have an adjusted R-squared of 40.2% and 42.4%, respectively.

Model 1 is inspired by the best OLS model proposed in this paper to predict R_C given the eight individuals, where H20 and VBS were added (also considering a quadratic relationship for Clay). In model 2, the Density was removed because it is strongly insignificant due to the constraint imposed on the mixtures to respect a density of 1. Model 3 tests the causal impact of SiO_2/Al_2O_3 on R_C, which is strongly correlated to Ip and OM (statistically significant here) according to the third part of the PCA analysis. Finally, Ip is removed in Model 4 to limit collinearity bias with OM and SiO_2/Al_2O_3, demonstrated as statistically significant in Model 3. According to model 4 in Table 4, three main significant parameters positively influence R_C, which are Blaine (at a 1% level of confidence), SiO_2/Al_2O_3 (at 1%), and VBS (at 1%). Specifically, a unit change in Blaine rises R_C by 7.851, 0.999 for SiO_2/Al_2O_3, and 0.498 for VBS. In opposition, OM negatively impacts R_C where an increase of 1 unity of it decreases R_C by 2.79×10^{-5}. Finally, Clay first negatively affects R_C (at 1%) until a turning point where the effect becomes positive. The squared of the Clay variable indicates that a unit change increases R_C by 0.402.

Table 4: OLS results (35 individuals)

VARIABLES	Model1 R_C	Model2 R_C	Model3 R_C	Model4 R_C
Clay	-1.835***	-1.869***	-1.890***	-1.904***
	(0.445)	(0.367)	(0.381)	(0.325)
Clay_sqr	0.374***	0.379***	0.402***	0.402***
	(0.0617)	(0.0497)	(0.0505)	(0.0476)
VBS	-0.282***	-0.263***	0.534**	0.498***
	(0.0902)	(0.0852)	(0.203)	(0.0972)
Blaine	7.517***	7.235***	7.791***	7.851***
	(2.232)	(1.748)	(1.794)	(1.825)
H2O	26.32	26.28	26.43	26.41
	(16.42)	(16.03)	(16.07)	(15.73)
OM	-2.23e-05**	-2.16e-05**	-2.62e-05**	-2.79e-05**
	(9.07e-06)	(8.07e-06)	(9.76e-06)	(1.04e-05)
SiO2	-0.0667**	-0.0744***		
	(0.0270)	(0.0101)		
Ip	-0.0112***	-0.0125*	-0.00230	
	(0.00329)	(0.00678)	(0.0128)	
Density	0.564			
	(1.550)			
SiO2_Al2O3			1.073*	0.999***
			(0.568)	(0.341)
Constant	-2.136	-0.786	-9.924*	-9.657**
	(6.986)	(3.543)	(5.213)	(4.270)
Observations	35	35	35	35
Adjusted R-squared	0.381	0.404	0.402	0.424
F-Stat	191.5	191.5	191.5	191.5
Prob > F	0	0	0	0

Robust standard errors in parentheses: *** p<0.01, ** p<0.05, * p<0.
Source: author's calculations.

3. CONCLUSION

In this work, two conclusions emerge from the various sediment samples studied. First of all, based on the study of the eight types of sediments characterized by various resistance to compression; the results demonstrate the importance of the physical properties of the sediments. More precisely, the Blaine, Density, and Clay are highlighted as positive determinants of R_C. In a certain measure, results also seem to corroborate the literature by showing the role of sediments' chemical properties. The Ip, OM, and SiO_2 are non-significant determinants in our model, but the PCA analysis highlights a strong correlation between these parameters, which may explain their non-significance when put together. Moreover, one limitation of the study is the very restricted sample size, so it is challenging to approach reality accurately. Finally, H_2O and alkali reagents (NaOH and Na_2SiO_3) do not appear in the results, as they are considered constant according to the previously described mix design.

Secondly, the eight types of sediments and 27 mixtures were studied together to understand better which mechanical and chemical properties influence compressive strength. In these estimates, activators of geopolymerization (SiO2/Al2O3 and OM) are statistically significant, with a negative impact for the first one and a negative for the latter. As expected, H_2O is not far from the 10% significance level. Finally, Blaine, Clay, and VBS are determinants for R_C. Unfortunately, the predicted power of the model is about 43% because the sample is limited and, more specifically, not normally distributed. Indeed, the 27 mixtures were first to respect a mass of 1, and then the optimal formulation was fixed according to Pauillac properties.

The last model, although promising, is ultimately limited by the sample size and its non-randomly character. Further investigations should consider a larger sample of random individuals, different by their chemical and physical properties, with varying mortars size to have more robust and better predictions. In conclusion, this work represents the first essential step in this research question and offers many fruitful perspectives.

4. AKNOWLEDGMENTS

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